

2-2 AND 2-3 INTERCOMBINATION TRANSITIONS IN BE-LIKE IONS

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Abstract

We report here on calculation of probabilities of intercombination transitions $2s^2\ ^1S_0$ - $2s2p\ ^3P_1$, $2s3p\ ^3P_1$ for Be-like ions along the isoelectronic sequence for large range of Z . Our results obtained with the $1/Z$ expansion method agree well with experimental data including the recent ones.

1. Introduction

Intercombination, or spin-forbidden, transitions are due to deviations from the pure LS-coupling. Since their very existence, at least for small nuclear charges Z , is a consequence of the subtle relativistic spin-orbit interaction, the agreement between theoretical and experimental results is an important measure of our understanding of atomic structure and interactions. In addition, intercombination lines are very important for plasma diagnostics, for example, in astrophysics and tokamak studies [8].

Since spin-forbidden transitions for not too large Z are much weaker than spin-allowed ones, the reliable determination of their transition probabilities requires serious experimental efforts. Recently two important experiments on measurement of the intercombination transitions probabilities in Be-like ions were carried out. Kwong *et al* [19] have improved their ion trap experiment on the transition $2s^2\ ^1S_0$ - $2s2p\ ^3P_1$ 1909 Å in C III and obtained the value of $121 \pm 7\ s^{-1}$ which differs considerably from the preliminary result of the same group $75\ s^{-1}$ [26]. In another experiment Granzow *et al* [14] have measured the probability of the $2s^2\ ^1S_0$ - $2s3p\ ^3P_1$ transition in Na VIII – Si XI ions. Similar measurements for smaller nuclear charges Z from N IV to Ne VII [9,15] were done more than ten years ago, so it is possible now to compare theoretical predictions along larger interval of Z . These two latest experimental works initiated a wave of theoretical calculations [11,13,3,28,12] where most sophisticated and elaborated up to now methods were used, e.g. multiconfiguration Hartree-Fock (MCHF), multiconfiguration Dirac-Fock

(MCDF), configuration interaction (CI) methods, multiconfiguration relativistic random-phase approximation (MCRRPA). In this paper we report the results of calculations of $2s^2\ ^1S_0 - 2s2p\ ^3P_1$ and $2s^2\ ^1S_0 - 2s3p\ ^3P_1$ transition probabilities along [Be] isoelectronic sequence by the Z expansion method. This approach is known to be very accurate in determination of energy levels of few-electron multicharged ions but as we will see in what follows gives also good results for intercombination probabilities.

In these calculations we use the MZ code [25] based on the perturbation theory on $1/Z$ parameter. The main principles of this approach and the code structure are well described in [25] so we refer the reader to this book for details.

2. Results and Discussion

Both intercombination transitions studied in this paper arise from mixing of triplet terms with the singlet ones. This mixing not only makes the spin-forbidden transition to be possible but also influences the level energies. Therefore the correspondence between the experimental and theoretical energies is an additional important check for accuracy of the calculations. Earlier the MZ method was successfully applied for calculation of the level energies for configurations $1s^22l'nl''$ ($n = 2, 3, 4$) of Na VIII - S XIII ions [24,1]. These references contain detailed examination of energy calculations by MZ so here we immediately pass to the discussion of obtained results. Here we calculated energies for configurations $2l'2l''$ and $2l'3l''$ for $Z = 6 - 26$. In most cases the difference between calculated in this work and experimental [17] energies is of order of a few units of 10^{-4} or less which is typical for calculations with the MZ code. For intercombination transitions two energy differences, namely $\Delta E(^3P_1 - ^1S_0)$ and $\Delta E(^1P_1 - ^3P_1)$, play a crucial role since these quantities explicitly enter the formula for transition probability in the first order of perturbation theory. In fact, our results for these energies have the highest accuracy except of the latest variational calculations [29]. Note that experimental energies for levels $2s2p\ ^3P_1$ ($Z = 18 - 26$) have a stable non-depending on Z shift of $\sim 350\text{ cm}^{-1}$ comparing to our results. Since all these energies were determined from the same experiment [4], it is quite possible that there was a systematic error in those measurements.

Until now only four experiments on measurement of $2s^2\ ^1S_0 - 2s2p\ ^3P_1$ transition probability were carried out, that is for C III [19], Fe XXIII [5], Kr XXXIII [6] and Xe LI [21]. The best known in this list is the widely used in solar plasma diagnostics intercombination line 1909 \AA in C III which has been discussed in many theoretical papers (see references in Ref. [27]). As we have noted above, the recently reported experimental results on C III [19] do not overlap with the previous measurements of the same group for this transition probability [26]. The new value $A_{CIII} = 121 \pm 7\text{ s}^{-1}$ agrees well with our result 120 s^{-1} and MCRRPA value of 118 s^{-1} [3] but contradicts the latest CI [11], MCHF [13] and MCDF [28] calculations which give 104 ± 4 , 103 ± 3 , and $100.3 \pm 4\text{ s}^{-1}$ respectively. As one can see from Fig. 1, the agreement between MZ probabilities and available data for Fe, Kr and Xe is also good. In addition to above mentioned CI, MCDF, MCHF, and MCRRPA calculations, we show on this Figure the extensive MCDF calculations for Be-like ions up to Xe LI [2], model potential results [20] and MC calculations with SUPERSTRUCTURE code [22] as well. Although different theoretical results give practically the same both Z -dependence and absolute values of probabilities for large $Z \geq 26$, the situation for small nuclear charges is not very clear yet and new accurate measurements for $Z < 10$ would be of great importance.

On Fig. 2 the theoretical and experimental results for transition probability $A(2s^2\ ^1S_0 - 2s3p\ ^3P_1)$ for $Z = 7 - 26$ are shown. At present there are old experimental data for $Z = 7 - 9$ [9], $Z = 10$ [15] and latest data for $Z = 11 - 14$ [14]. The theoretical results on Fig. 2 include MCDF [12], MCHF [7], CI [16] and HF-with-relativistic-corrections [10] calculations. As was shown by Fritzsche and Grant [12], for small Z the MCDF

method is rather slow convergent with increase of the number of configurations included. This is probably to be a reason for large discrepancy between that paper and results of Kim *et al* [18]. It is seen from Fig. 2 that different theoretical approaches show again similar Z -dependence, except for smallest Z , where more accurate measurements would be desirable. The new experimental results by Granzow *et al* [14] seem to give Z -dependence rather different from theoretical one, although in sufficiently narrow region. At least for Na VIII the value of A is considerably larger than most recent theoretical results. This feature needs further investigation, especially since the authors claim that this value appears to be an overestimate.

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1. Ando, K. et.al., 1992, *Phys. Scr.*, **46**, 107.
2. Cheng, K.T. et.al., 1979, *At. Data Nucl. Data Tables* **24**, 111.
3. Chou, H.-S. et.al., 1994, *Chin. J. Phys.* **32**, 261.
4. Dere, K.P., 1978, *Astrophys. J.* **221**, 1062.
5. Dietrich, D.D. et.al., 1978, *Phys. Rev. A* **18**, 208.
6. Dietrich, D.D. et.al., 1980, *Phys. Rev. A* **22**, 1109.
7. Ellis, D.G., 1983, *Phys. Rev. A* **28**, 1223.
8. Ellis, D.G. et.al., 1990, *Comm. At. Mol. Phys.* **22**, 241.
9. Engström, L. et.al., 1979, *Phys. Scr.* **20**, 88.
10. Fawcett, B.C., 1985, *At. Data Nucl. Data Tables* **33**, 479.
11. Fleming, J. et.al., 1994, *Phys. Scr.* **49**, 316.
12. Fritzsche, S. and Grant, I.P., 1994, *Phys. Scr.* **50**, 473.
13. Froese Fischer, C., 1994, *Phys. Scr.* **49**, 323.
14. Granzow, U. et.al., 1994, *Phys. Scr.* **49**, 148.
15. Hardis, J.E. et.al., 1983, *Phys. Rev. A* **27**, 257.
16. Hibbert, A., 1979, *J. Phys. B* **12**, L661.
17. Kelly, R.L., 1987, *J. Phys. Chem. Ref. Data*, **16**, Suppl. 1.
18. Kim, Y.-K. et.al., 1988, *J. Opt. Soc. Am. B* **5**, 2215.
19. Kwong, V.H.S. et.al., 1993 *Astrophys. J.* **411**, 431.
20. Laughlin, C. et.al., 1978, *J. Phys. B* **11**, 2243.
21. Möller, G. et.al., 1989, *Z. Phys. D* **11**, 333.
22. Nussbaumer, H. and Storey, P.J., 1979, *J. Phys. B* **12**, 1647.
23. Safronova, U.I. and Senashenko, V.S., 1982, *Phys. Scr.*, **25**, 37.
24. Safronova, U.I. et.al., 1990, *Optics and Spectroscopy* **68**, 151.
25. Shevelko, V.P. and Vainshtein, L.A., 1993, *Atomic Physics for Hot Plasmas* (IOP Publishing Ltd., Bristol).
26. Smith, P.L. et.al., 1984, *Phys. Scr.* **18**, 88.
27. Träbert, E., 1993, *Phys. Scr.* **48**, 699.
28. Ynnerman, A. and Froese Fischer, C., 1995, *Phys. Rev. A*, **51**, 2020.
29. Zhu, X.-W. and Chung, K.T., 1994, *Phys. Rev. A* **50**, 3818.

Fig. 1. Scaled transition probabilities for $2s^2\ ^1S_0 - 2s2p\ ^3P_1$ line in Be-like ions. *Experiment*:
 • Z=6 [19], Z=26 [5], Z=36 [6], Z=54 [21]; *Theory*: — this paper, \triangle [20], \diamond [22], \dots
 [2], + [11], \times [13], --- [3], \square [28].

Fig. 2. Scaled transition probabilities for $2s^2\ ^1S_0 - 2s3p\ ^3P_1$ line in [Be] ions. *Experiment*: •
 Z=7-9 [9], Z=10 [15], Z=11-14 [14]; *Theory*: — this paper, \triangle [16], \diamond [7], --- [12],
 \dots [10].



